Scientific Support Group Overview

During the reorganization of the ALS at the end of 1997, two new user support groups were created: the User Services Group (discussed later in this Compendium, in the User Services section) and the Scientific Support Group. The Scientific Support Group (SSG), headed by Zahid Hussain with John Bozek as deputy, consists of a team of scientists, postdocs, students, and associate beamline scientists. The primary role of the SSG is to provide scientific and technical support to ALS users. The nature of that support ranges from technical assistance in operating the beamlines or experimental equipment to full collaboration with the users' groups. The scientific staff of the SSG are all experienced synchrotron radiation users (at the ALS as well as at other facilities) who are familiar with many of the beamlines, experimental endstations, and techniques, as well as the scientific problems that can be addressed using the capabilities of the ALS. SSG members continue to assist ALS users in developing their research programs by helping in the preparation of grant proposals for new funding and in the development of new experimental equipment. A major thrust in this area over the past year has been the development of Beamline 10.0.1 and its associated endstations for high-resolution electron spectroscopy in solids and gases, described in detail below. Also, an effort is currently underway to develop a set of user-friendly data analysis tools to provide a "seamless computing environment" for working with experimental data acquired at the ALS.

Increased User-Friendliness and Experimental Efficiency

Members of the group are fully or partially responsible for the operation and development of several of the facility's beamlines, including Beamlines 1.4, 7.0.1, 8.0.1, 9.3.1, 9.3.2, 10.0.1, 10.3.1, and 10.3.2. Increasing the "user-friendliness" of these beamlines while maintaining their efficiency and effectiveness is one of the major goals of the group. To this end, the first mirror and entrance slit of Beamline 8.0.1 were replaced with internally cooled versions similar to those installed in Beamlines 7.0.1 and 10.0.1. The new mirror and slit were required to handle the high heat load from the undulator at small gap settings. The beamline can now be used with a 14-mm gap even at the top of the fill with no degradation in performance. The slits were also modified to have electrically isolated jaws, allowing the installation of a feedback loop on the first mirror to keep the beam centered on the entrance slit. Several additional improvement projects were initiated in 1998 to make several of the beamlines more user friendly. Computer control of the entrance and exit slits of the spherical grating monochromator (SGM) beamlines (7.0.1, 8.0.1, 9.3.2, and 10.0.1) is being developed to minimize errors in setting the slits as well as to provide the capability to carry out constant-bandwidth photon energy scans. Tilt sensors are being incorporated into the SGMs as calibration constants that will reduce the photon energy calibration shift observed when changing gratings. A motor-driven horizontal-deflecting-mirror positioning system is being implemented on Beamline 10.0.1 to minimize the time required for alignment when switching between endstations. Nonbeamline improvements include the development of a Laue back-diffraction system for crystal alignment (with the gracious donation of space on the Physical Biosciences diffractometer in Building 80) and replacement of the sample manipulator on the x-ray photoelectron diffraction (XPD) chamber.

Communication and Outreach

The SSG strives to maintain and further develop communications with ALS users to build and improve the scientific program. Workshops are held occasionally to identify new areas of opportunity. Outreach is also a goal of the SSG to broaden the user base of the ALS. Group members often attend and organize meetings and conferences to publicize the capabilities of the ALS to many different scientific communities.

Beamline 1.4

Infrared (IR) spectromicroscopy research at Beamline 1.4 was led by SSG member Michael C. Martin and included a wide variety of topics. This beamline came into full operation in June 1998 and has rapidly developed a broad user community. In a collaboration with other Berkeley Lab scientists, led by H. Holman, IR absorption signals from individual human cells were observed to change as a specific gene was expressed in response to environmental toxins. This observation could lead to an exciting new method for quickly measuring exposures as well as determining risk-based standards for pollutant levels. Some of the same researchers also used the IR microscopy beamline to show that specific microbes found in a toxic waste site are able to bioremediate toxic Cr (VI) compounds by reducing them to safe Cr (III) compounds. Three more research groups focused on processes in the environment: T. Raab from the University of Colorado, Boulder, began studies of the interactions between plant roots and soils in the rhizosphere; and two groups, one from the University of Delaware, led by D. Sparks, and one from Carnegie-Mellon University, led by U. Ghosh, investigated the chemistry of soils and the kinetics and mechanisms of ion sorption to soil components. Two groups from U.C. Berkeley round out the highlighted experiments for this beamline. One, led by R. Glaeser, is using IR microscopy to monitor the photocycle of bacteriorhodopsin microcrystals with the ultimate goal of doing protein crystallography on another ALS beamline to determine the atomic structure of each conformation this protein goes through. A second, led by R. Saykally, is finding signs of deeply supercooled water using liquid microjets; they hope to probe liquid water at lower temperatures than have been possible to date.

Beamline 7.0.1

The Beamline 7.0.1 angle-resolved photoemission endstation is run by SSG member Eli Rotenberg. This endstation has been optimized for high-flux, high-resolution, angle-resolved photoemission. In addition, wide flexibility in scan types (photon energy vs. sample orientation, for example) and sample preparation techniques have been and continue to be developed to cater to user needs. Some examples of work done or published in 1998 include the following:

- **Photoemission of engineered magnetic nanostructures.** The creation of a continuum of samples on a single crystal allowed systematic studies of electron standing-wave formation as a function of quantum well structure. The most important aspects of these experiments were the small photon spot size (~50 μm)[1] and an *in-situ* sample preparation facility for the creation of double-wedged nanostructures.[2]
- **Resonant photoemission study of α and δ plutonium.** The electronic structure of various phases of plutonium metal are of tremendous interest, not only because of applications to environmental cleanup, but also because plutonium straddles the line between having localized and delocalized f electrons. Los Alamos National Laboratory scientists, together with the ALS, developed a dedicated sputter/anneal chamber to prepare clean samples and thereby enable safe transfer to the nonradioactive sample analysis chamber. (Contacts: Jeff Terry and Roland Schulze, Los Alamos National Laboratory)
- **Valence-band photoemission of icosahedral quasicrystals.** We developed a sample preparation technique for sputter/annealing AlPdMn alloy quasicrystals. Conventional valence-band angle-resolved photoemission reveals electronic bands (similar to conventional metals) with icosahedral point-group symmetry. This experiment takes advantage of the high photon flux due to the relatively low cross section of the features (<10% of total electron density participating). (Contacts: Eli Rotenberg, Advanced Light Source, or Karsten Horn, Fritz-Haber Institute, Berlin)

[1]Kawakami, R.K. et al., *Phys. Rev. Lett.* **80**, 1754 (1998).
[2]Kawakami, R.K. et al., *Nature* **398**, 132 (1999).

Beamline 10.0.1

Two projects supported by the Department of Energy's 1996–1998 Scientific Facilities Initiative (SFI) necessitated the creation of a new beamline at the ALS with high spectral resolution in the 20- to 350-eV photon energy range. The new beamline, Beamline 10.0.1, was built using many existing components. The spherical grating monochromator (SGM) from Beamline 9.0.1 was moved to become the heart of Beamline 10.0.1. New vacuum components and optics were constructed as required to replace parts left in the shared regions of the previous beamline. A new 4.5-m-long, 10-cm-period undulator was constructed for the beamline. Permanent magnets, a support and drive system, and even a vacuum tank were salvaged from other projects and used in the construction of the new undulator for Beamline 10.0.1. The horizontal focusing of the beamline was changed through the installation of new mirrors to provide a 100-μm focus in one of the side branches of the beamline. Construction of the beamline proceeded rapidly following the shutdown of Beamline 9.0.1 in March 1998. Beam was passed into the new beamline in June 1998, at the end of the machine shutdown for installation of the new U10 undulator. The new endstations (described below) provided by the SFI funds are permanently installed on two branches of the beamline. A third large, permanent endstation for studying the photoionization of ions is installed on the third branch with space for temporary endstations provided.

High-Energy-Resolution Spectrometer (HERS)

Highly correlated electron systems such as the d- and f-band materials offer both intellectual challenges in physics and prospects for novel materials applications. Such systems, which include high-temperature superconductors and heavy-fermion and Kondo systems, are not adequately described by either atomic physics or one-electron band theory. Photoemission is an ideal tool to study highly correlated electron systems and has the potential to have a major impact on our understanding of these materials. In this collaborative effort between the spokesperson for the project, Z.X. Shen (Stanford University), members of the SSG, and the Mechanical Engineering Group, a state-of-the-art High-Energy-Resolution-Spectrometer (HERS) for angle-resolved photoemission experiments at the ALS was developed to study highly correlated electron systems. The heart of the experimental station is a state-of-the-art angle-resolved electron-energy analyzer (Scienta SES-200) mounted on a chamber that rotates about the photon beam axis. The combination of this analyzer, a high-precision low-temperature sample goniometer, and the use of Beamline 10.0.1 allows the performance of ultrahigh-energy and -momentum-resolution photoemission experiments. Also under construction is a high-efficiency electron-spin detector that will allow the determination of all three components of electron spin with high energy resolution, comparable to kT.

High-Resolution Angle-Resolved Photoemission Study of Highly Correlated Electron Systems. Systematic study of high-temperature superconductors using HERS is providing new insight into these fascinating materials. An ultrahigh-momentum-resolution photoemission study of a Bi2212 sample indicates that the superconducting transition is not merely the opening of a gap due to an effective attractive interaction between the well-defined quasiparticles in the normal state, but rather, these quasiparticles themselves are only formed upon lowering the temperature below T_c.

The stripe phase first proposed to explain neutron data from Nd-substituted $La_{1.28}Nd_{0.6}Sr_{0.12}CuO_4$ (Nd-LSCO) represents a new paradigm for charge carriers in a solid. Unlike in conventional metals, where the charge distribution is homogeneous, the stripe phase envisages microscopic antiferromagnetic domains separated by one-dimensional domain walls (stripes) consisting of hole carriers and frustrated spins. The implication of this charge segregation propensity on the conduction as well as the superconducting mechanism is at the heart of the current debate in high-T_c research today. So far, much of the stripe information stems from interpretation of the incommensurate neutron scattering peaks. Very little is known about the electronic structure of these materials. Angle-resolved photoemission has been applied to directly probe the electronic structure and charge dynamics of the stripe phase. Results indicate the existence of one-dimensional charge confinement. For details, see X.J. Zhou et al. in this compendium.

High-Resolution Atomic and Molecular Electron Spectrometer (HiRAMES)

The complexities of electronic structure in atoms and molecules are often only made clear when highly differential spectra are obtained. A high-resolution atomic and molecular electron spectrometer (HiRAMES) built with funding from the Scientific Facilities Initiative was designed and constructed by N. Berrah (Western Michigan University) with the assistance of the SSG. The endstation was constructed using a state-of-the-art Scienta SES-200 electron-energy analyzer mounted on a chamber that rotates about the photon beam axis. Gaseous samples are introduced into a gas cell mounted on the end of the electron lens with differentially pumped openings for the photon beam and a slit allowing electrons to leave the cell in the direction of the analyzer. Sample pressures as high as 10^{-4} Torr are isolated from the ultrahigh vacuum requirements of the beamline by windowless differential pumping. An oven has also been developed to provide a beam of low-volatility materials (i.e., metal atoms) for photoionization studies.

Atomic and Molecular Photoelectron Spectroscopy. The valence and inner-shell electron emission spectra of atoms and simple molecules offer the opportunity to study a variety of electronic structure phenomena in ideal noninteracting systems. With the assistance of SSG member John Bozek, the atomic, molecular, and optical (AMO) physics program at the ALS is targeting the fundamental understanding of many-body phenomena in the simplest systems (atoms and molecules) where full quantum-mechanical calculations can be compared with the experimental results. For example, high-resolution C 1s photoelectron spectra of the simple hydrocarbon molecule C_2H_2 have resolved the symmetry splitting of the two carbon 1s levels ($1\sigma_u$ and $1\sigma_g$), making it possible to experimentally identify the symmetry channel of the above-edge resonance.[1] Resonant Auger electron spectra of carbon monoxide, CO, have been measured with vibrational resolution for the excitation and vibrational resolution of the subsequent deexcitation. The resulting spectra highlight the dynamics of deexcitation of the inner-shell excitation (C $1s \rightarrow 2\pi^*$) by probing the vibrational excitation of the final-state ion.[2] High-resolution electron spectra of the S 2p levels of carbonyl sulphide (OCS) exhibit nine lines due to vibrational and molecular field splitting. The molecular field splitting removes the degeneracy of the S $2p_{3/2}$ level and provides a means of accessing the fundamental amplitudes and phase shifts associated with the transition matrix element.[3]

[1]Thomas, T.D. *et al*., *Phys. Rev. Lett.* **81**, 5776 (1998).
[2]Kukk, E., J.D. Bozek, and N. Berrah, *J. Chem. Phys*., in press.
[3]Kukk, E., J.D. Bozek, N. Berrah, J.A. Sheehy, and P.W. Langhoff, *Phys. Rev. Lett.*, submitted.

Beamline 10.3.1

The scientific program of the microprobe beamline, Beamline 10.3.1, has been very active thanks to the efforts of SSG member Scott McHugo. Semiconductor research is taking off both for solar cells and integrated circuit semiconductors; silicon is the major research material, with GaAs also showing potential. Groups involved include S. Martinuzzi’s group in France, E.R. Weber’s group from U.C. Berkeley, the National Renewable Energy Laboratory (NREL) in Colorado, Astropower in Delaware, Bayer Solar in Germany, and Mitsubishi Silicon in Oregon. T. Cahill’s research group (U.C. Davis) has been investigating particulates from the upper atmosphere. D. Sayers’ group (North Carolina State) has used the microprobe to study cancerous lung tissue from the Chernobyl area.

In a major revitalization effort, the data acquisition system for the microprobe is being updated using funds from the Berkeley Lab's Center for X-Ray Optics. The new system will allow greater control over the speed of the scanning (rastering the sample through the microfocused beam) and will allow multiscanning. Areas of interest can be quickly defined using the short dwell times available in the new system, saving a considerable amount of setup time. The multiscanning feature allows spectra to be accumulated until the appropriate signal-to-noise level is achieved, unlike the previous system, which required guessing at the appropriate dwell time. The dead time has also been decreased in the new software, resulting in improved throughput. Finally, the data analysis software has been improved for ease of visualization and to improve users' ability to quickly disseminate their data.